

PUBCHEM_54605649

40730-78-7 | DTXSID90714109

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -10.7 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.65e-01

Confidence level: 6.14e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2,5-Furandione

Measured: -11.8

Predicted: -11.7

[Image not found](#)

2-Methyl-p-benzoquinone

Measured: -10.6

Predicted: -10.7